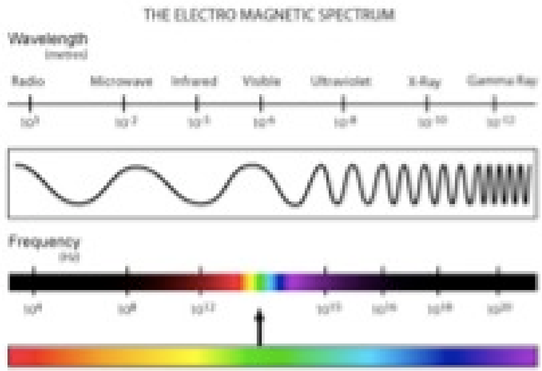


$c = \lambda \nu$

c = speed of light
3×10^8 m/s

ν = frequency
waves per second

λ = wavelength

1

Constructing electronic structure of a hydrogen atom

Part I:

energy of radiation can be estimated by its frequency

$$\nu = \frac{c}{\lambda}$$

ν: frequency of radiation
c: velocity of radiation
λ: wavelength of radiation

ν(unit = s^{-1})
λ(unit = nm ; 1 nm = 1 x 10^{-9} m)
c = 3 x 10^8 m s^{-1} / :300,000km

$$E = h\nu$$

E : energy of radiation
h : Planck constant
ν: frequency of radiation

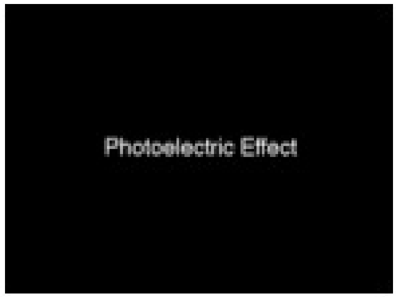
E(unit = J)
h = 6.626 x 10^{-34} Js

2

Photoelectric effect:

The energy of an electron is proportional to the frequency of light given off.

The experiment:



3

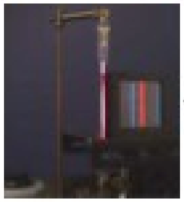
Because each element has a different number of electrons, each element gives off characteristic wavelengths, or colors.

When electrons are excited, they increase in energy. When they drop down to their original location, they give off energy equal to the difference between the 2 locations.

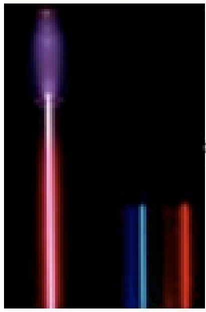
So, the color of the flame tells us something about the energy levels the electrons occupied.

4

We can excite hydrogen atoms by running an electric current through hydrogen gas......



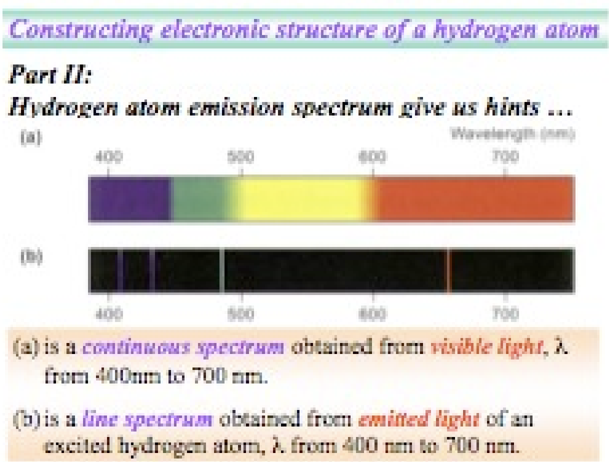
And then viewing the glowing gas through a **spectroscope**



The result is the visible **hydrogen spectrum**:

5

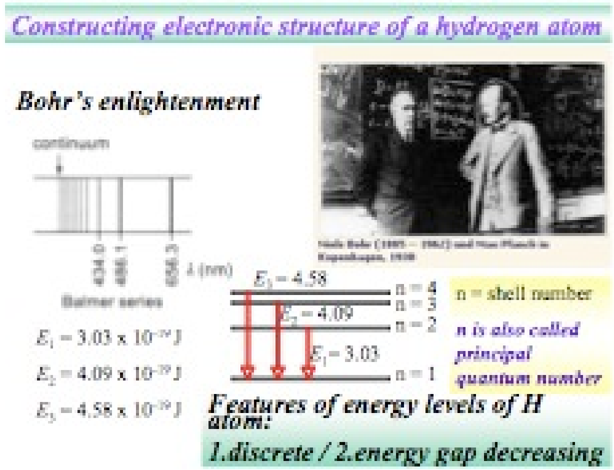
This can give us a picture of the hydrogen atom:



The H atom emits light at **discrete energy levels**.

6

Niels Bohr discovered that H's lone electron emits light in the discrete levels seen in the hydrogen spectrum:



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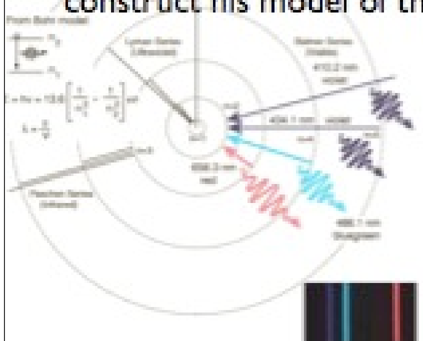
Bohr used this concept of **energy levels** to construct his model of the hydrogen atom:



Features of Bohr's model:

Electrons occupy discrete energy levels, or "shells"

The energy gap decreases as the shell number increases

8

So if hydrogen's spectrum can tell us about the structure of a H atom, can the spectra of other elements help us create models of those atoms?

http://jersey.uoregon.edu/vlab/elements/Elements.html

What do we notice about the spectra of the other elements?

They are more complex than H

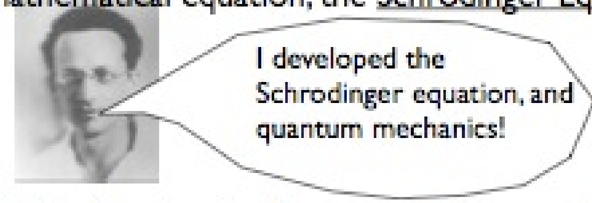
In general, their complexity increases as atomic number increases

The Bohr Model **does not** work for elements other than Hydrogen.

Atomic spectra just get too complicated to be explained by the Bohr Model.

So, a new model must be created to explain the atomic structure of **all** the elements, not just hydrogen!

Enter Schrodinger used **probability** to express the location of an electron in an atom by developing a mathematical equation, the Schrodinger Equation.

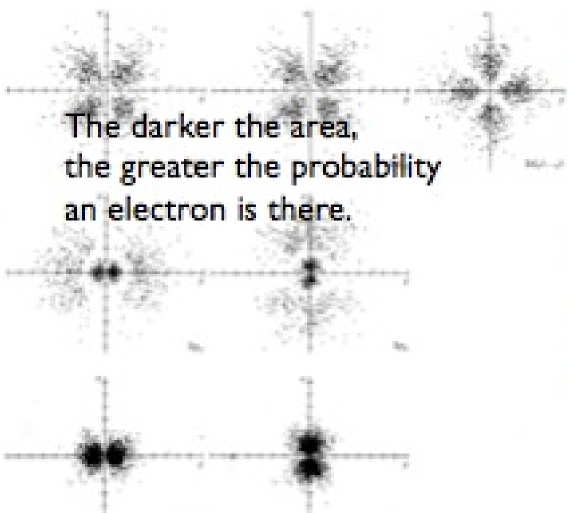


This led to the development of the **quantum mechanical model** of the atom.

Let's compare the **Bohr model** with the **quantum mechanical model.**

11

Characteristics of the quantum mechanical model:

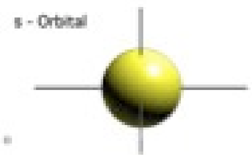


The location of electrons are given by the probability of finding them in that area. These areas have different energy levels.

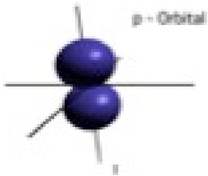
These probability regions are called **atomic orbitals**.

12

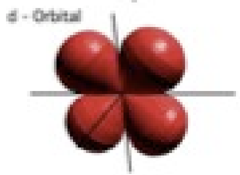
These orbitals have the following shapes:



each can contain 2 electrons
Groups 1 and 2 on the periodic table



each can contain 6 electrons
Groups 3-8 on the periodic table



each can contain 10 electrons
transition metals on periodic table

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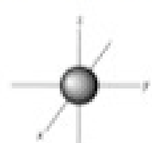
Energy levels of electrons are denoted by principal quantum numbers (n). n = 1, 2, 3, 4, etc.

Each energy level, n, may have energy sublevels, each corresponding to an orbital of a different shape.

Principal energy level	Number of sublevels	Type of sublevel
n=1	1	1s (1 orbital)

2 max e-



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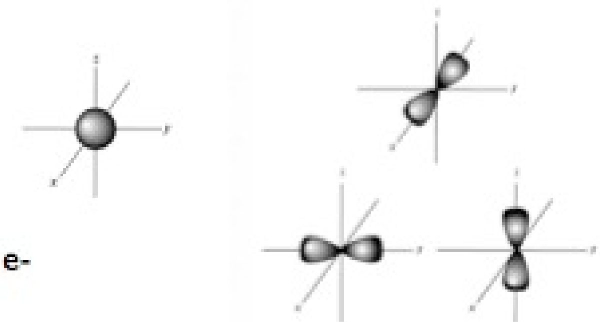
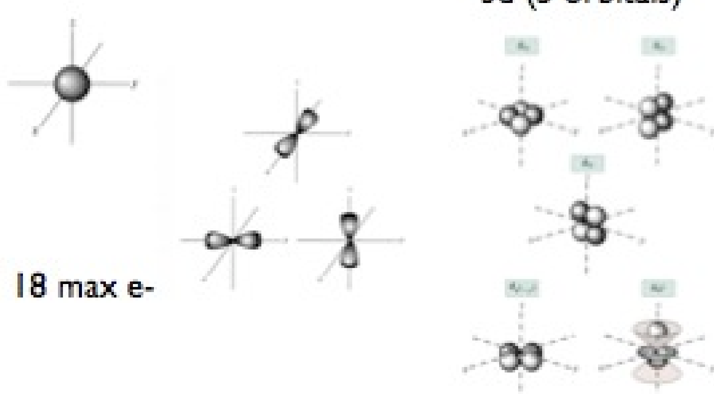
Principal energy level	Number of sublevels	Type of sublevel
n=2	2	2s (1 orbital), 2p (3 orbitals)



8 max e-

15

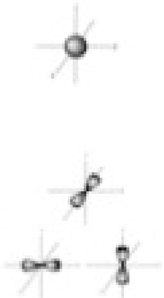
Principal energy level	Number of sublevels	Type of sublevel
n=3	3	3s (1 orbital), 3p (3 orbitals) 3d (5 orbitals)

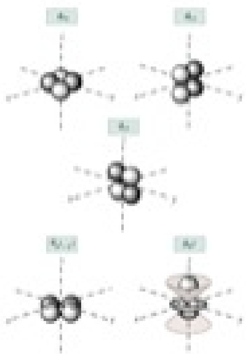


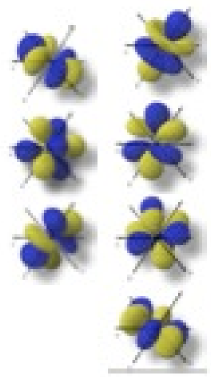
18 max e-

16

Principal energy level	Number of sublevels	Type of sublevel
n=4	4	4s (1 orbital), 4p (3 orbitals) 4d (5 orbitals),4f (7 orbitals)







32 max e-

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Three rules tell you how to find the electron configuration:

Aufbau principal: e- occupy orbitals of the lowest energy level first.

Pauli exclusion principal: an atomic orbital may describe at most 2 e-. Each has a different spin: clockwise and counterclockwise.

[↑↓]

Hund's rule: e- occupy orbitals 1 at a time, with the same spin direction, until all are filled. Only then will e- be paired with another of opposite spin.

[↑↓]	[↑↓]	[↑↓]	[↑↓]	[↑↓]
1s	2s	$2p_x$	$2p_y$	$2p_z$

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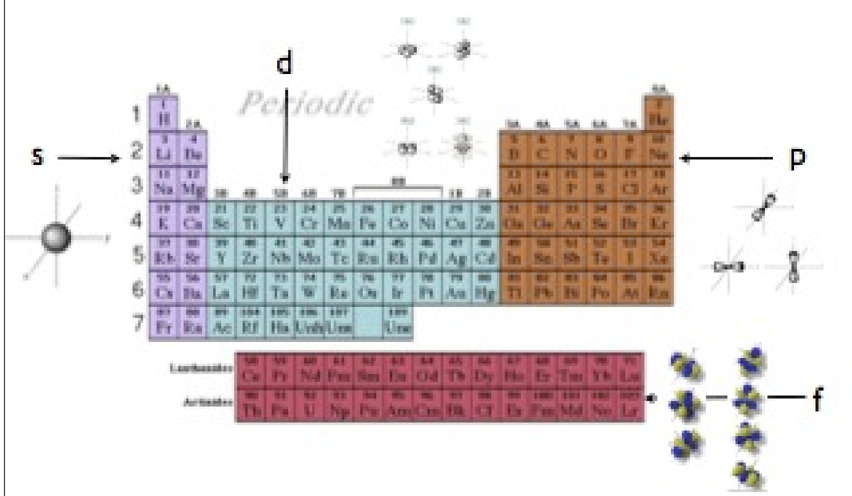
How do we write electron configurations for each element?



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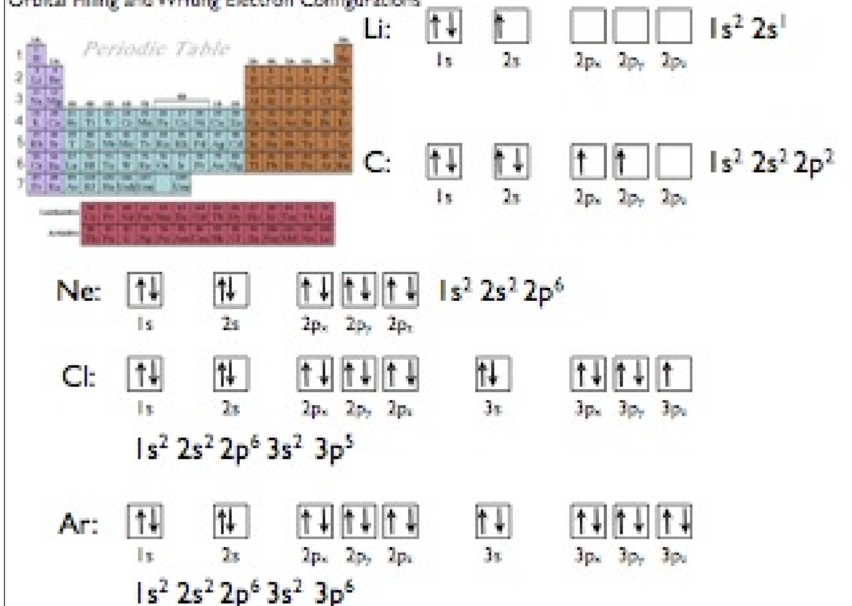
Orbital Filling and Writing Electron Configurations



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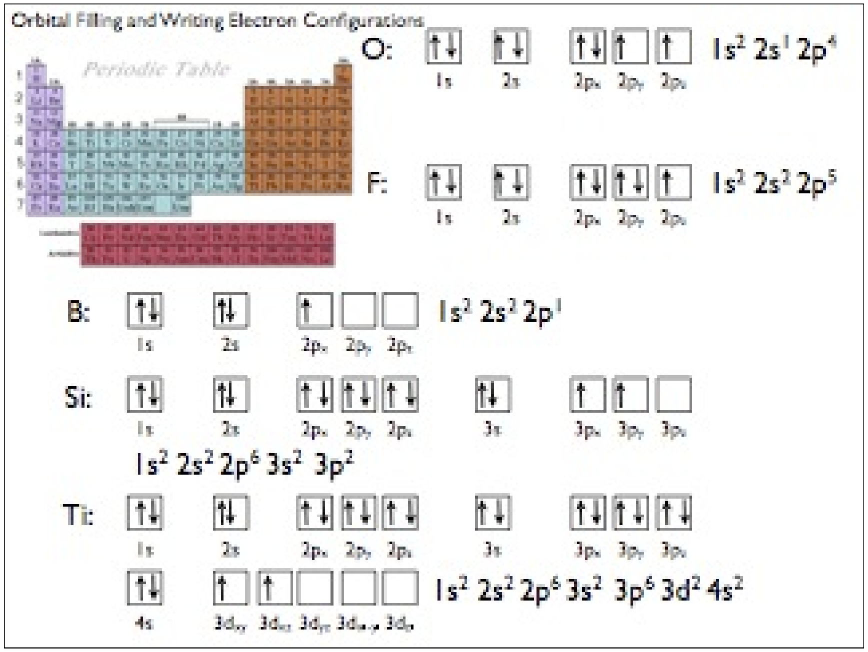
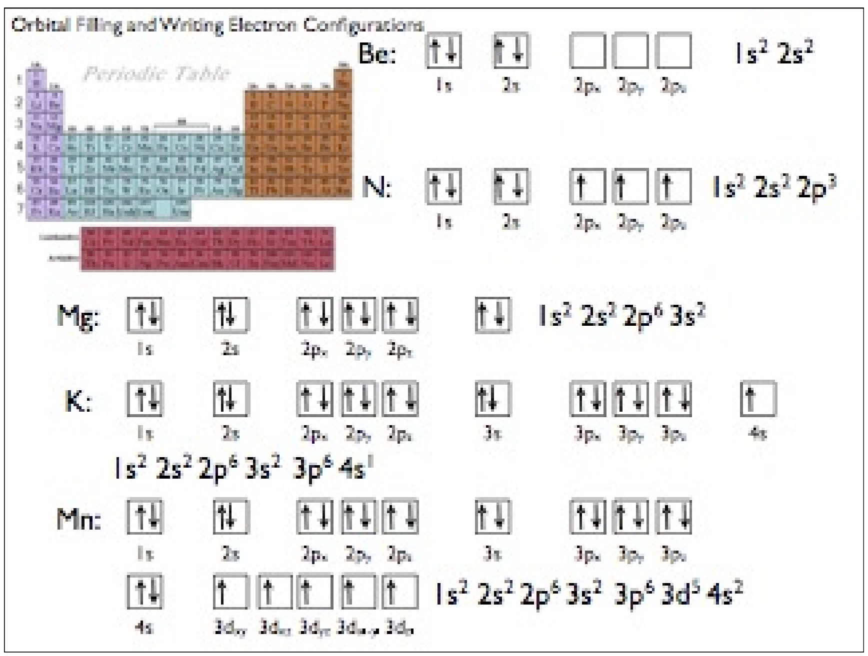

Orbital Filling and Writing Electron Configurations
Periodic Table
O:
1s 2s 2px 2py 2pz
1s² 2s¹ 2p⁴
F:
1s 2s 2px 2py 2pz
1s² 2s² 2p⁵
B:
1s 2s 2px 2py 2pz
1s² 2s² 2p¹
Si:
1s 2s 2px 2py 2pz 3s 3px 3py 3pz
1s² 2s² 2p⁶ 3s² 3p²
Ti:
1s 2s 2px 2py 2pz 3s 3px 3py 3pz
4s 3dxy 3dxz 3dyz 3dx²-y² 3dz²
1s² 2s² 2p⁶ 3s² 3p⁶ 3d² 4s²

21


Orbital Filling and Writing Electron Configurations
Periodic Table
Be:
1s 2s 2px 2py 2pz
1s² 2s²
N:
1s 2s 2px 2py 2pz
1s² 2s² 2p³
Mg:
1s 2s 2px 2py 2pz 3s
1s² 2s² 2p⁶ 3s²
K:
1s 2s 2px 2py 2pz 3s 3px 3py 3pz 4s
1s² 2s² 2p⁶ 3s² 3p⁶ 4s¹
Mn:
1s 2s 2px 2py 2pz 3s 3px 3py 3pz
4s 3dxy 3dxz 3dyz 3dx²-y² 3dz²
1s² 2s² 2p⁶ 3s² 3p⁶ 3d⁵ 4s²

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Let's review electron configurations and write them:

Copper and chromium have configurations that are exceptions to the Aufbau Principle:

	Expected configuration:	Actual configuration:
Cr:	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \underline{3d^4\ 4s^2}$	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \underline{3d^5\ 4s^1}$
Cu:	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \underline{3d^9\ 4s^2}$	$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ \underline{3d^{10}\ 4s^1}$

Having half-filled or filled 3d orbitals is more stable than a filled 4s orbital.

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So what is quantum mechanics, really?

It describes the motions of electrons and other subatomic particles as waves.

Electrons move as waves? Aren't they particles???

Davisson and Germer, at Bell Labs in NJ, did an experiment that showed that electrons behave as waves!

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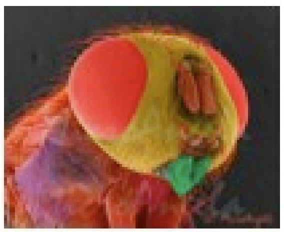
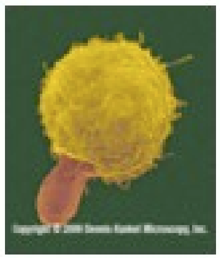
Since electrons behave as waves, they can be used to magnify objects, much like light can....only much smaller objects!

electron microscope

Electron microscope images:





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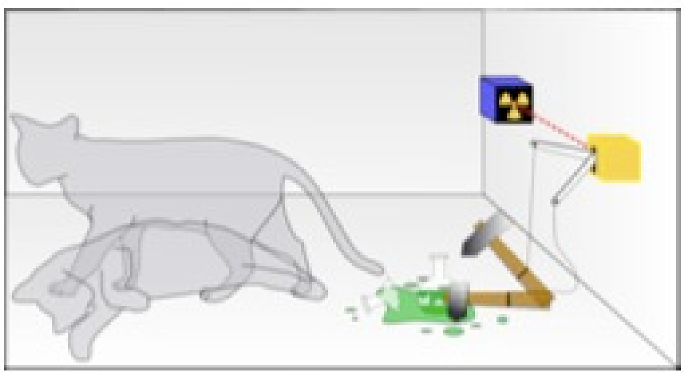

Schrödinger's Cat: A cat, along with a flask containing a poison, is placed in a sealed box shielded against environmentally induced quantum decoherence. If an internal Geiger counter detects radiation then the flask is shattered, releasing the poison which kills the cat. Quantum mechanics suggests that after a while the cat is simultaneously alive *and* dead. Yet, when we look in the box, we see the cat *either* alive *or* dead, not a mixture of alive *and* dead.

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